

Program to Optimize Simulated Trajectories II (POST2) Surrogate Models for Mars Ascent Vehicle (MAV) Performance Assessment

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LIST OF ACRONYMS AND SYMBOLS

| | |
|------|---|
| ACO | Advanced Concepts Office |
| DOE | design of experiments |
| MAV | Mars Ascent Vehicle |
| PMF | propellant mass fraction |
| POST | Program to Optimize Simulated Trajectories II |
| RSE | response to surface equation |
| Sol | Martian solar day |
| TW | thrust-to-weight |

NOMENCLATURE

| | |
|-----------------|------------------------|
| I_{sp} | specific impulse |
| m_b | burnout mass |
| m_p | propellant mass |
| R | response |
| x | input parameter |
| β | regression coefficient |

TECHNICAL MEMORANDUM

PROGRAM TO OPTIMIZE SIMULATED TRAJECTORIES II (POST2) SURROGATE MODELS FOR MARS ASCENT VEHICLE (MAV) PERFORMANCE ASSESSMENT

1. INTRODUCTION

Trajectory optimization is a key component in assessing launch vehicle performance during conceptual design. For prephase A and phase A concept definition studies, the Integrated Space Transportation Team within Marshall Space Flight Center's Advanced Concepts Office (ACO) implements Program to Optimize Simulated Trajectories II (POST2). POST2 is an industry-standard tool that implements a direct solution method to approximate the control function for an optimal trajectory.¹ Successfully employing POST2 for a trade study requires a trajectory expert in the loop to ensure that the control variables remain within the feasible space and produce acceptable trajectories.² For this reason, trade studies can only be as broad as the trajectory expert's time will allow. A very limited number of cases can be completed by hand in a given workday.

In an attempt to alleviate the execution time issues associated with POST2 and allow for much broader trade space exploration, ACO has developed a tool for automating ascent trajectory optimization. This tool captures heuristics developed over years of analyst experience and leverages the power of modern computing to speed up the evaluation of large sets of vehicle trajectories. The basic premise of the tool, known as multiple Programs to Optimize Simulated Trajectories, or multiPOST, is to use multiprocessing to simultaneously evaluate random repetitions for a single vehicle case. The analysis-based heuristics are then used to help converge to acceptable trajectories or reject unrealistic ones. The approach implemented in multiPOST is detailed further in references 3 and 4.

Although primarily used by ACO for Earth-to-orbit vehicle studies, multiPOST is capable of executing POST2 for nearly any valid vehicle input deck. Using this flexibility, multiPOST was applied to carry out a Mars Ascent Vehicle (MAV) study. The MAV is a key component to successful human exploration of Mars and is being considered within NASA's evolvable Mars campaign.⁵

The primary focus of this MAV study was to use multiPOST to investigate the effects of mass fraction, liftoff location, and propulsion on the payload mass delivered to a particular orbit by a two-stage ascent vehicle. The stages of the vehicle contain the propulsion related elements, such as engines and propellant tanks. The payload mass in this case was the crew cabin, which included the crew and provisions for the trip from the surface of Mars to rendezvous with the Mars-Earth transportation vehicle. The ultimate goal was to minimize the MAV gross mass for a given cabin mass. Any changes in the MAV mass will impact the sizing of other architecture elements including Earth launch and in-space transportation as well as entry, descent, and landing.⁶

2. APPROACH

The primary purpose of the multiPOST tool is to enable the execution of much larger sets of vehicle cases to allow for broader trade space exploration. However, this exploration is not achieved solely with the increased case throughput. The multiPOST tool is applied to carry out a Design of Experiments (DOE), which is a set of cases that have been structured to capture a maximum amount of information about the design space with minimal computational effort. The results of the DOE are then used to fit a surrogate model, ultimately enabling parametric design space exploration.

The approach used for the MAV study includes both DOE and surrogate modeling. First, the primary design considerations for the vehicle were used to develop the variables and ranges for the multiPOST DOE. The final set of DOE variables were carefully selected in order to capture the desired vehicle trades and take into account any special considerations for surrogate modeling.

Next, the DOE sets were executed through multiPOST. Following successful completion of the DOE cases, a manual verification trial was performed. The trial involved randomly selecting cases from the DOE set and running them by hand. The results from the human analyst's run and multiPOST were then compared to ensure that the automated runs were being executed properly. Completion of the verification trials was then followed by surrogate model fitting.

After fits to the multiPOST data were successfully created, the surrogate models were used as a stand-in for POST2 to carry out the desired MAV trades. Using the surrogate models in lieu of POST2 allowed for visualization of vehicle sensitivities to the input variables as well as rapid evaluation of vehicle performance. Although the models introduce some error into the output of the trade study, they were very effective at identifying areas of interest within the trade space for further refinement by human analysts.

The next section will cover all of the ground rules and assumptions associated with DOE setup and multiPOST execution. Section 3.1 gives the final DOE variables and ranges, while section 3.2 addresses the POST2 specific assumptions. The results of the verification trials are given in section 4. Section 5 gives the surrogate model fitting results, including the goodness-of-fit metrics for each fit. Finally, the MAV specific results are discussed in section 6.

3. GROUND RULES AND ASSUMPTIONS

3.1 Design of Experiments

Primary design considerations for the MAV include mission parameters such as surface location and destination orbit as well as vehicle parameters such as propulsion and vehicle masses. At this point in the MAV design, mass fractions are more appropriate due to the lack of detailed subsystem masses. Using a Propellant Mass Fraction (PMF) allows the analysis to be more flexible and to capture many unique vehicle configurations as long as they fit within the bounds of the study. The PMF for this study was defined for each stage as:

$$\text{PMF} = m_p / (m_p + m_b) , \quad (1)$$

where m_p is stage usable propellant mass, and m_b is stage burnout mass. The PMFs do not include any mass attributed to the crew cabin.

In addition to stage PMF, other vehicle parameters were added to the DOE to represent the MAV propulsion system. In order to capture many potential propulsion system types, continuous parameters were used for engine thrust and specific impulse (I_{sp}). The ranges for thrust and I_{sp} were developed to capture potential propellant combinations for the MAV (e.g. liquid oxygen/liquid methane, nitrogen tetroxide/monomethyl hydrazine). This allowed the analyst to dial values representing specific types of propulsion into a single surrogate model.

The variable for number of engines is discrete, which requires special treatment. Due to the discrete nature of this variable, the DOE sets were split to improve the ease of fitting surrogate models. Discrete parameters typically cause difficulty in achieving acceptable fits, therefore a single surrogate is fit to each discrete dataset. It is important to note that the number of engines only applies to the first stage of the vehicle. It was assumed for this study that the second stage would always contain a single engine. This engine is assumed to be identical in thrust and I_{sp} to the engines on the first stage.

Two mission parameters of interest were included in the study DOE. First, the destination orbits for the MAV were defined based upon current Mars orbit rendezvous options at 1 Sol and 5 Sol.⁶ These orbit options are discrete; however, they were represented using a continuous parameter for the required reserve delta-v. The ranges shown in table 1 for reserve delta-v were developed to capture orbit options under consideration for the MAV. The second mission parameter, latitude, is a continuous variable representing the liftoff location. Since no specific landing sites were identified for the study, the latitude range was set to capture a large number of landing sites that have been identified for consideration.⁷ The final set of DOE inputs and ranges for the two-stage MAV can be seen in table 1.

Table 1. DOE inputs and ranges for two-stage MAV.

| Input Variable | Min | Max |
|--------------------------------|-------|-------|
| No. of engines (discrete) | 2, 3 | |
| Reserve delta-V (m/s) | 1,200 | 1,800 |
| Liftoff latitude (°) | 0 | 60 |
| Thrust per engine (kN) | 68 | 200 |
| Engine I_{sp} (s) | 300 | 460 |
| Stage 1 PMF | 0.75 | 0.95 |
| Stage 2 PMF | 0.65 | 0.9 |
| Payload (crew cabin) mass (kg) | 1,800 | 5,000 |

3.2 Program to Optimize Simulated Trajectories II Assumptions

The POST2 input deck used common assumptions for the Martian environment. The gravitational model for Mars comes from the 1997 Astronomical Almanac.⁸ The atmospheric data was taken from the Space and Planetary Environment Criteria Guidelines for Use in Space Vehicle Development.⁹ The reference area for MAV aerodynamics was set at 22.06 m² with the speed of sound input as 487.89332 m/s.⁶

The POST2 input deck was set up to fly to an initial orbit of 100 by 250 km while reserving an excess delta-v required to transition to a higher target orbit. The excess delta-v required was set as the variable dvmarr in the deck.

The dependent variables in the POST2 input deck defined the target orbit using geocentric radius, flight path angle, and inertial velocity. Independent variables for optimization consisted of seven pitch rates, launch azimuth, initial weight of the payload, and throttle level for a throttling event during ascent. The throttle level was constrained to a minimum of 20%.

The first pitch event occurs at 5 s into the ascent, followed by a gravity turn at 45 s. Between the end of the gravity turn and insertion into the initial orbit, six additional pitch events occur. The gravity turn is ended by the first stage reaching zero propellant. At this point, the first stage is jettisoned, and the second stage begins thrusting at its optimized throttle level.

The final main-engine cutoff for the two-stage vehicle occurs when the MAV achieves its initial orbit of 100 by 250 km. Simultaneously, the MAV is constrained to have a remaining delta-v equal to the excess amount required to reach the final target orbit.

4. VERIFICATION

Using the variables and ranges in table 1, a DOE was executed through the multiPOST tool. Random cases were then selected from the DOE to test the multiPOST execution of the MAV POST2 deck. These cases were extracted from the results and individually checked by a POST2 expert. It is expected that the POST2 expert will beat multiPOST in most cases. If any large differences ($>3\%$) in output are noticed during these checks, the setup and execution of the automated deck is investigated. Table 2 shows payload comparisons for a representative set of cases from the MAV study.

Table 2. MultiPOST versus manual payload comparison.

| Manual Payload (kg) | Automated Payload (kg) | Delta-V (Manual-Auto) (%) |
|---------------------|------------------------|---------------------------|
| 4,818.55 | 4,818.12 | 0.008 |
| 3,608.79 | 3,608.79 | 0 |
| 4,563.15 | 4,555.90 | 0.16 |
| 2,828.51 | 2,828.76 | -0.009 |
| 3,977.55 | 3,978.55 | -0.025 |
| 3,409.29 | 3,401.56 | 0.226 |
| 4,447.39 | 4,428.31 | 0.429 |
| 4,529.77 | 4,517.74 | 0.266 |
| 4,145.21 | 4,119.40 | 0.623 |
| 5,331.47 | 5,331.01 | 0.008 |
| 4,041.84 | 4,041.66 | 0.005 |
| 3,815.59 | 3,815.66 | -0.002 |

5. SURROGATE MODELING

5.1 Model Fitting in JMP

Following successful verification testing, surrogate models were fit for each of the discrete datasets. The statistical software JMP was used to complete the model fitting. This software provides tools for fitting many types of models including Gaussian processes, Kriging, neural networks, and response surface equations.^{10,11} Response Surface Equations (RSE) were selected as the desired model type for the MAV study due to their relative simplicity as compared to Gaussian process models or neural networks. Although the trajectory response space is typically multimodal and nonlinear, higher order RSEs have been used to successfully fit results from POST2 for other studies.³

RSEs are typically fit using the method of least squares to estimate the regression coefficients.¹² Equation 1 gives the generic form of a second order RSE, where R is the response, x terms are input parameters, and β terms are regression coefficients. Note that the model is linear in the β parameters and is therefore a linear regression model, regardless of the order of the input parameters¹²:

$$R = \beta_0 + \sum_{j=1}^k \beta_j x_j + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j + \sum_{j=1}^k \beta_{jj} x_j^2 . \quad (2)$$

As noted above, higher order RSE models have been successfully used to fit POST2 output data. However, as the order of the model is increased, the total number of terms in the equation also increases. Since $k + 1$ cases are required to regress the β coefficients for a model of k terms, this also increases the total number of DOE cases that must be completed through multiPOST. In order to keep the number of required cases as well as the overall length of the equation to a reasonable level, stepwise regression was utilized in JMP.

Stepwise regression uses a statistical significance level to determine which terms in the regression model are most beneficial to the model's ability to predict the data. During model fitting, terms are added or removed from the model based upon their calculated significance levels. The result is a model containing only terms that are statistically significant for predicting the response, which tends to be much more compact than the full model.

In addition to stepwise regression, k -folds cross validation was implemented when fitting the models in JMP. K -folds cross validation splits the full set of cases into k different sets or 'folds.' The model is fit to $k - 1$ sets of data, leaving the remaining set for model validation. After fitting a total of k models, the one with the best validation statistics is returned as the final model.¹⁰

5.2 Goodness-of-Fit Testing

When a surrogate model is returned, multiple goodness-of-fit tests are applied to accept or reject the fit. First, the coefficient of multiple determination, or R^2 , is used as an initial indicator of fit acceptability. The R^2 value is a measure of the reduction in variability of the response obtained from the model.¹² Based upon experience with fitting POST2 data, an R^2 value greater than 0.99 warrants further goodness-of-fit testing. Any value below 0.99 will require refitting after investigation of outliers or execution of additional DOE runs.

When fitting to POST2 data, the investigation of outliers tends to be the only action required to improve a fit. Although multiPOST utilizes heuristics to eliminate unreasonable trajectories, some of these trajectories can still pass along into the final data set. These cases are identified using the residual-by-predicted plot in JMP. This plot shows the predicted response value for each point plotted against its residual as compared to the actual response value. The desired shape of this plot is a ‘shotgun spread’ of points with no clear trends—an example of which is shown in reference 3. Any points that are significantly outside the main point cloud are tagged as outliers for further investigation.

Using the detailed POST2 output for each of the outliers, an analyst can easily determine whether or not the points can be excluded from the fit. Typically, these cases illustrate odd behavior, such as extreme lofting (affectionately dubbed a ‘rollercoaster’ trajectory) or very excessive pitch profiles due to a high thrust-to-weight (TW). Any case deemed to be unrealistic or unflyable for a crewed MAV is then removed from the model fitting dataset.

The final goodness-of-fit test is used to calculate the error percentage of the surrogate model across the entire dataset. This percentage encompasses both the points used to fit the model itself and the points held back for validation purposes. After calculating the error, the characteristics of the percent error distribution are used as a final acceptance check of the model. Typically, the mean is desired to be as close to zero as possible and the standard deviation must be below one. Figures 1 and 2 provide the final error distributions for the MAV surrogate models. Note that the error percentage was calculated based upon the difference between the surrogate model and the multiPOST output.

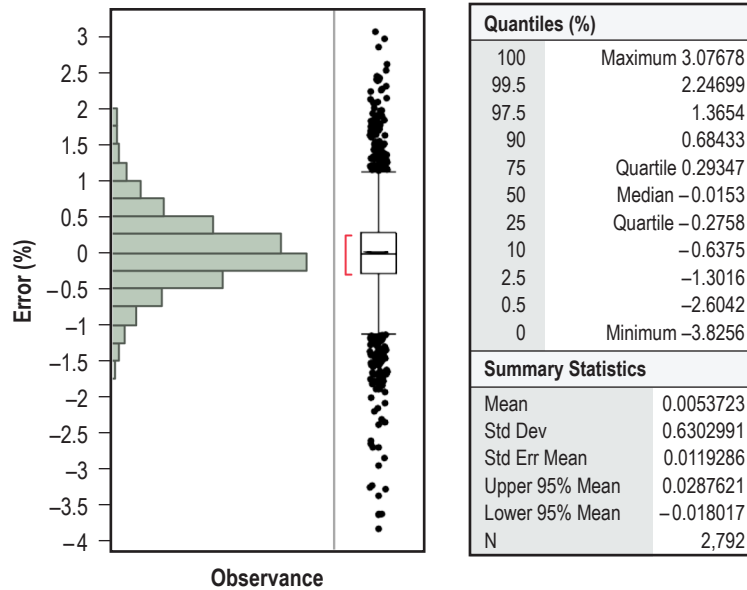


Figure 1. Percentage of error distribution for two-engine TSTO surrogate.

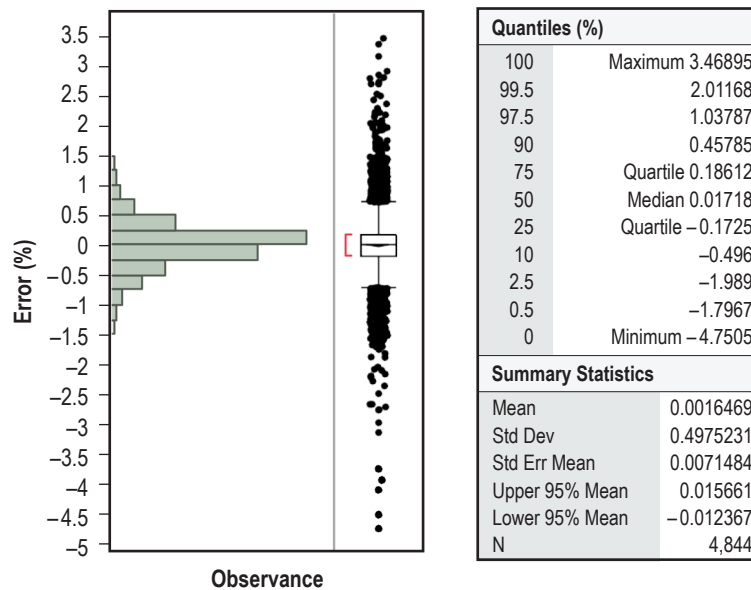


Figure 2. Percentage of error distribution for three-engine TSTO surrogate.

It is important to note that the resulting surrogate models are only valid within the bounds shown in table 1. Any case within the bounds that is evaluated through the surrogate will lie within the error distributions in figures 1 and 2. If any of the input variables entered into the surrogates are outside the bounds, the response of the surrogate is not valid, and it is highly likely that the percent error will be well outside of the distributions shown in the figures.

6. RESULTS

After performing goodness-of-fit testing and accepting the MAV surrogates, the equations were used to analyze trades of interest. As discussed in section 3, these trades include propellant types, crew cabin (payload) masses, and stage PMFs. Propellant types were represented by varying the engine thrust and I_{sp} . Multiple destination orbits were represented by fixing the excess delta-v input variable in the surrogate models. The excess delta-v values used for the specific orbits can be seen in table 3.

Table 3. Excess delta-v values for target orbits.

| Orbit | Excess Delta-V (m/s) |
|-------|-------------------------|
| 1 Sol | 1,434 |
| 5 Sol | 1,580 |

First, the sensitivity to liftoff latitude was analyzed for each target orbit. Figure 3 shows an example of the latitude sensitivity for a representative two-stage MAV flying to two different target orbits. As seen in the figure, increasing latitude increases the gross liftoff mass by approximately 2–3 metric tons over the entire range of latitude settings. This effect, however, is very small in comparison to the effects of thrust, I_{sp} , and stage PMF, which can affect gross mass by tens of tons over their respective ranges. Therefore, the latitude was fixed at the median value of 30° for the rest of the results within this section.

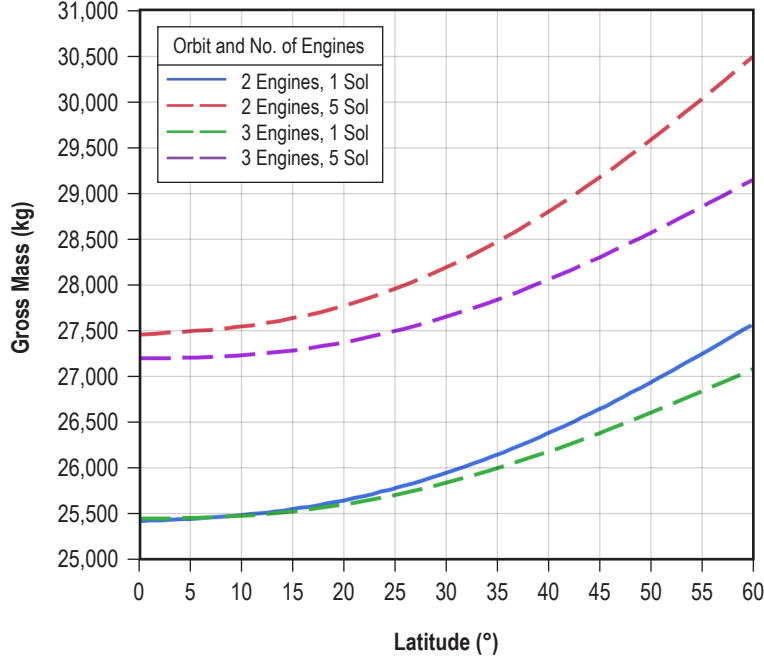


Figure 3. Liftoff latitude versus gross mass for two target orbits. Payload = 3 mt, I_{sp} = 360 s, thrust = 100 kN, stage 1 PMF = 0.85, and stage 2 PMF = 0.75.

After fixing latitude, a first set of figures was developed to investigate the optimal thrust level for the two-stage MAV with a given crew cabin mass. As discussed previously, the Mars mission architecture is very sensitive to the mass of the MAV. Optimizing the thrust level for a given payload will result in the smallest vehicle gross mass, thereby reducing the mass of the architecture.

To generate these figures, the thrust per engine was varied across the entire range noted in table 1 for both the two- and three- engine configurations. The PMFs for each stage were held constant using values representing a nominal MAV configuration. In figures 4–7, the first stage PMF was 0.8355, and the second stage PMF was 0.7639. The first stage PMF was 0.8507, and the second stage PMF was 0.7898 for figures 8–11. The variations in engine thrust were carried out at various I_{sp} settings, which are colored in each figure. Figures 4–7 used a fixed crew cabin mass of three metric tons, while figures 8–11 used four metric tons. From these figures, an optimal TW can be identified for a given orbit and I_{sp} .

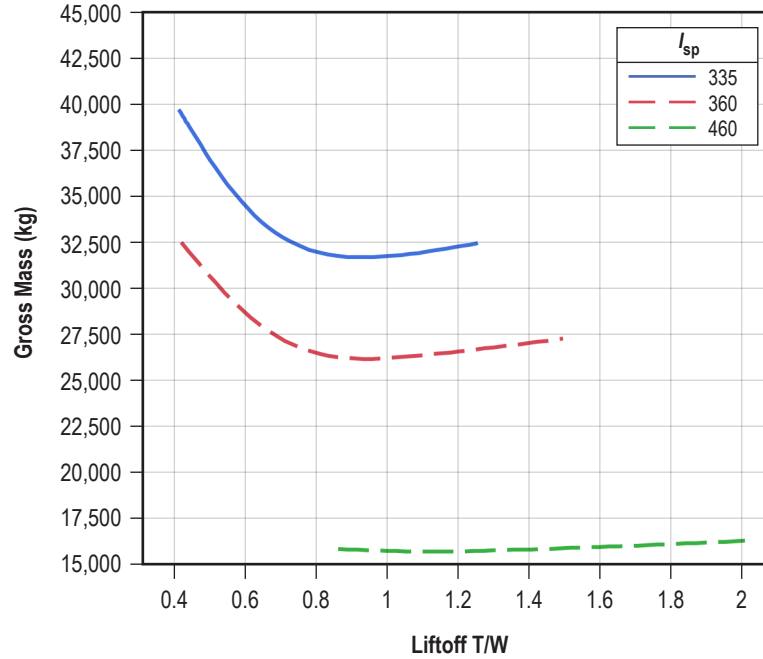


Figure 4. Liftoff TW versus gross mass for two-engine MAV with stage 1 PMF = 0.8355, stage 2 PMF = 0.7639, crew cabin mass = 3 mt, latitude = 30°, and orbit = 1 Sol.

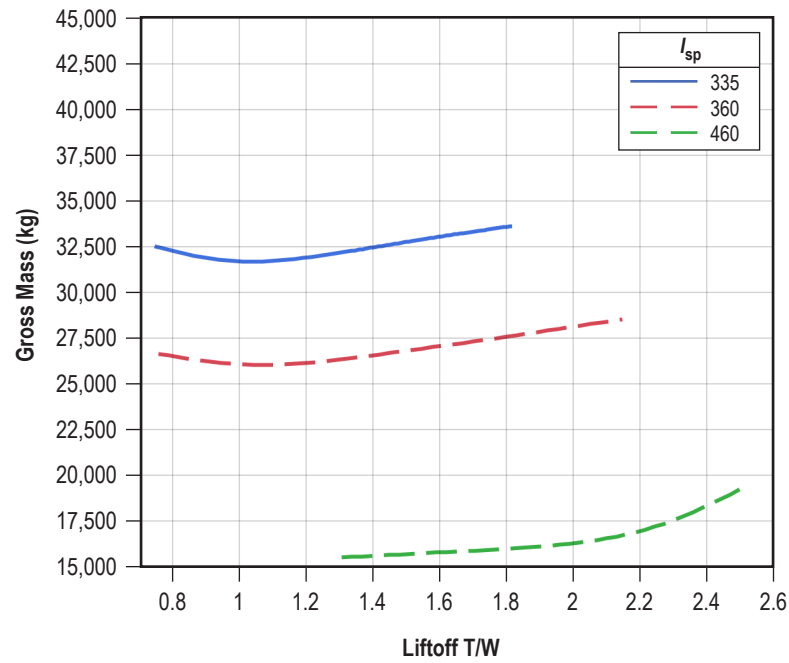


Figure 5. Liftoff TW versus gross mass for three-engine MAV with stage 1 PMF = 0.8355, stage 2 PMF = 0.7639, crew cabin mass = 3 mt, latitude 30°, and 1 Sol orbit.

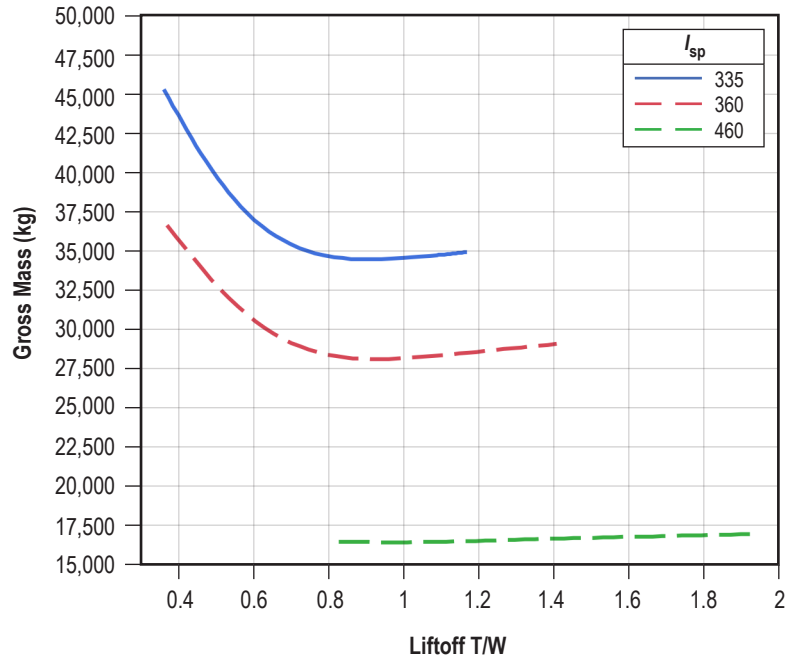


Figure 6. Liftoff TW versus gross mass for two-engine MAV with stage 1 PMF = 0.8355, stage 2 PMF = 0.7639, crew cabin mass = 3 mt, latitude = 30°, and orbit = 5 Sol.

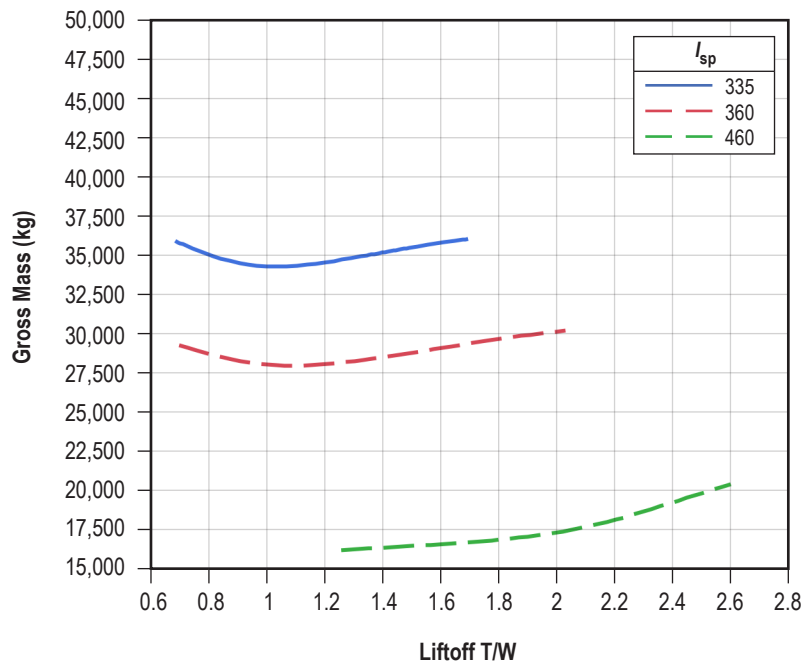


Figure 7. Liftoff TW versus gross mass for three-engine MAV with stage 1 PMF = 0.8355, stage 2 PMF = 0.7639, crew cabin mass = 3 mt, latitude = 30°, and orbit = 5 Sol.

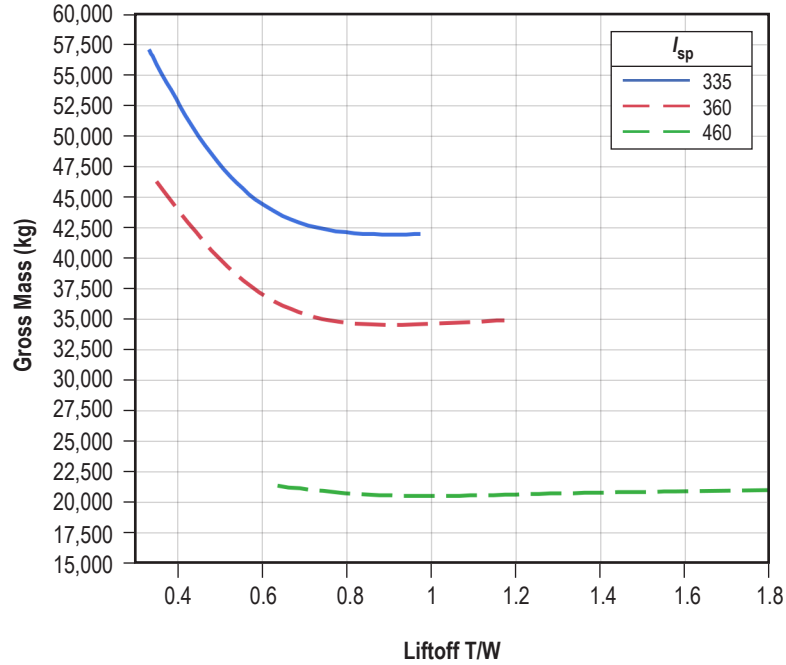


Figure 8. Liftoff TW versus gross mass for two-engine MAV with stage 1 PMF = 0.8507, stage 2 PMF = 0.7898, crew cabin mass = 4 mt, latitude = 30°, and orbit = 1 Sol.

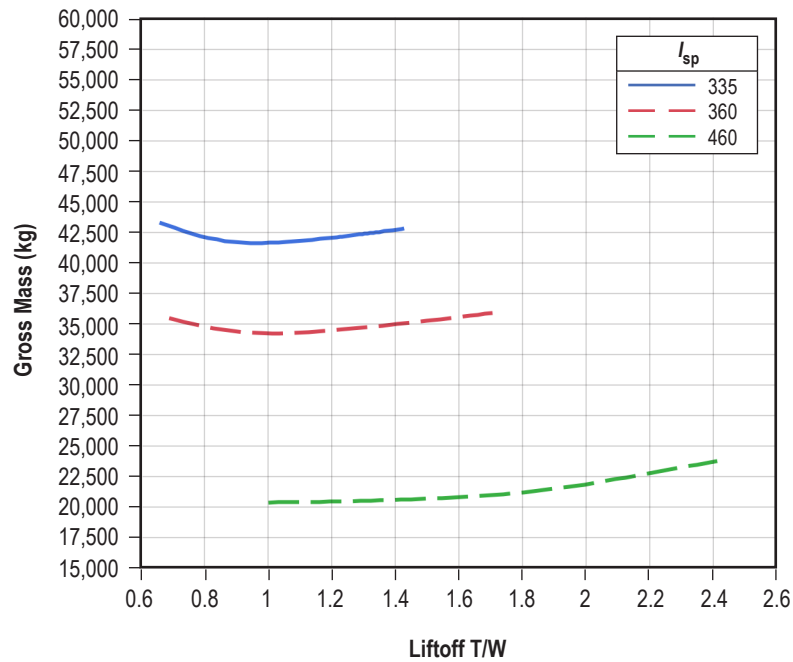


Figure 9. Liftoff TW versus gross mass for three-engine MAV with stage 1 PMF = 0.8507, stage 2 PMF = 0.7898, crew cabin mass = 4 mt, latitude = 30°, and orbit = 1 Sol.

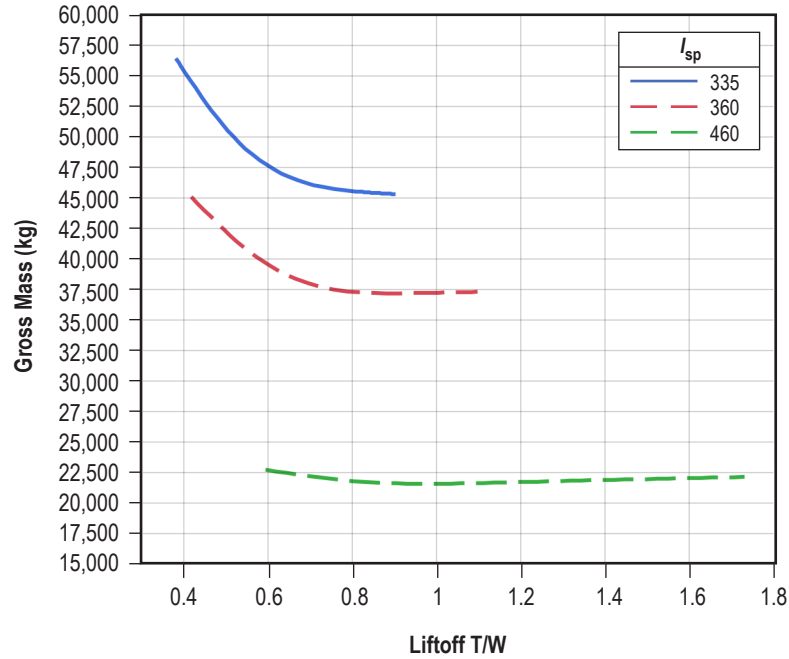


Figure 10. Liftoff TW versus gross mass for two-engine MAV with stage 1 PMF = 0.8507, stage 2 PMF = 0.7898, crew cabin mass = 4 mt, latitude = 30°, and orbit = 5 Sol.

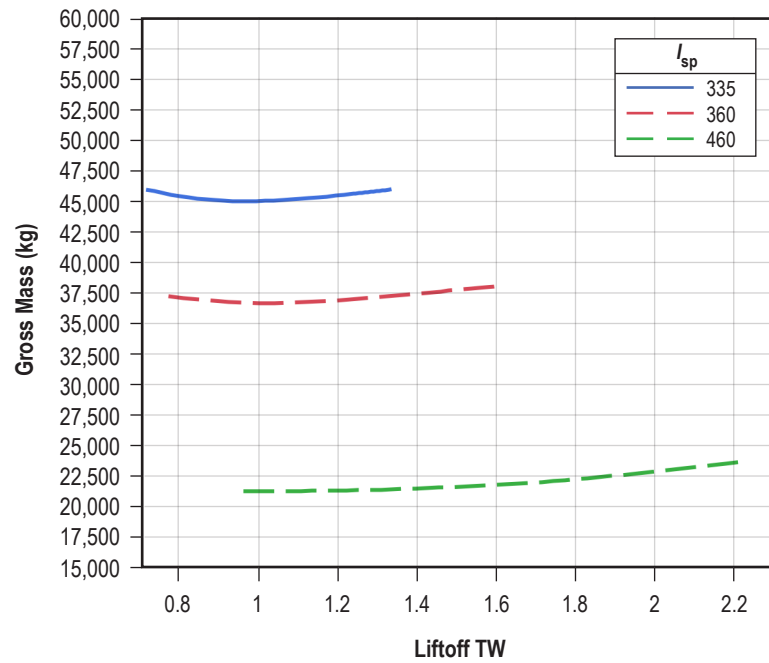


Figure 11. Liftoff TW versus gross mass for three-engine MAV with stage 1 PMF = 0.8507, stage 2 PMF = 0.7898, crew cabin mass = 4 mt, latitude = 30°, and orbit = 5 Sol.

Using the optimal TW information, a second set of figures was developed to investigate the effects of various stage PMF settings on vehicle gross liftoff mass and payload delivered. This was done by varying the PMF settings of the vehicle stages while maintaining a near-optimal TW. Therefore, the data in the second set of figures consists of vehicles with optimal thrust-to-weights that produce a minimum gross liftoff mass for a given crew cabin mass.

The PMF settings represented worst, nominal, and best cases for the two-stage MAV and are listed in table 4. Figures 12–14 and figures 15–17 illustrate the payload delivered versus gross liftoff mass for various I_{sp} and PMF assumptions for a 1 Sol and 5 Sol orbit, respectively.

Table 4. Stage PMF settings for figures 12–17.

| Setting Name | Stage 1 PMF | Stage 2 PMF |
|--------------|-------------|-------------|
| Low | 0.75 | 0.65 |
| Nominal | 0.85 | 0.75 |
| High | 0.95 | 0.85 |

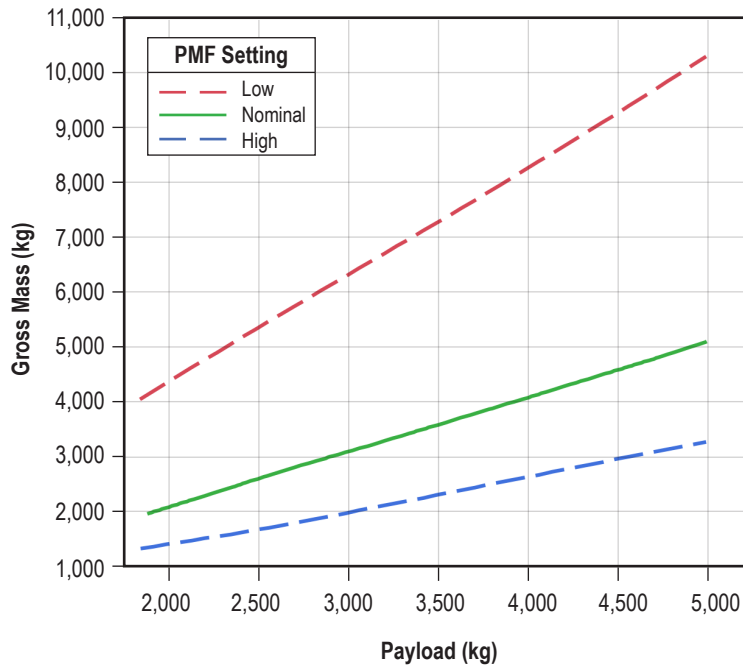


Figure 12. Payload versus gross mass for $I_{sp} = 335$ s, latitude = 30° , and orbit = 1 Sol.

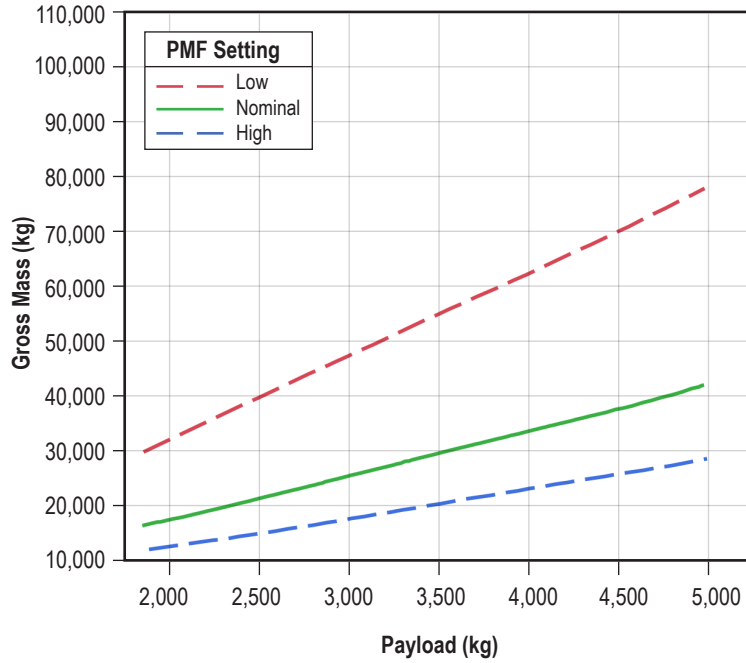


Figure 13. Payload versus gross mass for $I_{sp} = 360$ s, latitude = 30° , and orbit = 1 Sol.

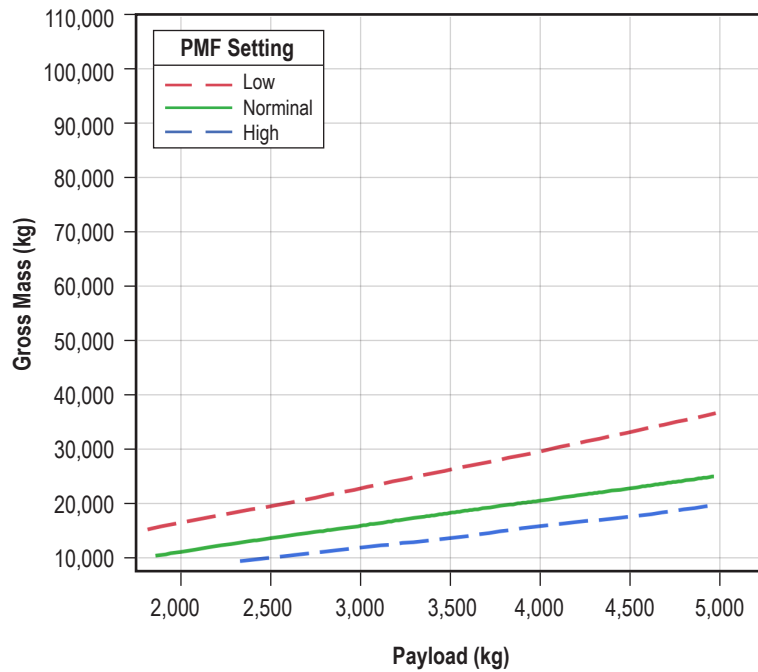


Figure 14. Payload versus gross mass for $I_{sp} = 460$ s, latitude = 30° , and orbit = 1 Sol.

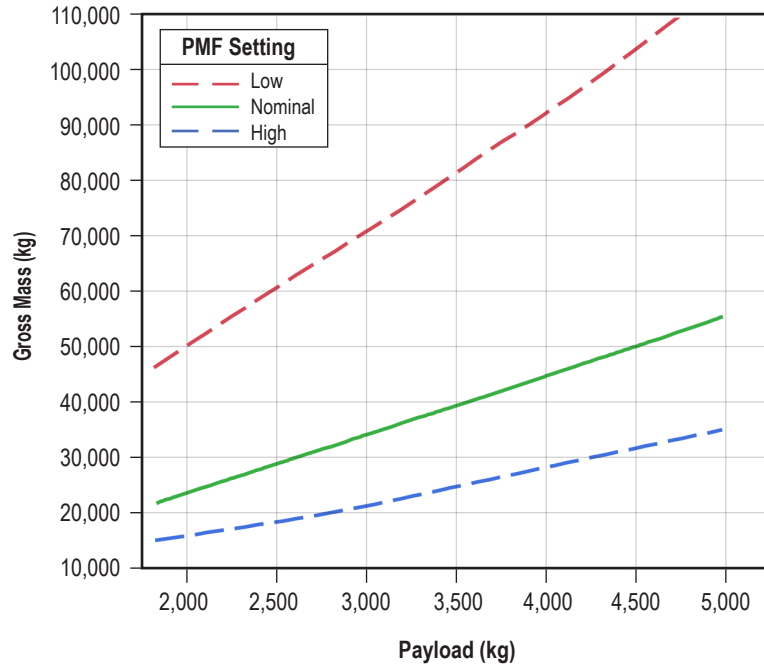


Figure 15. Payload versus gross mass for $I_{sp} = 335$ s, latitude = 30° , and orbit = 5 Sol.

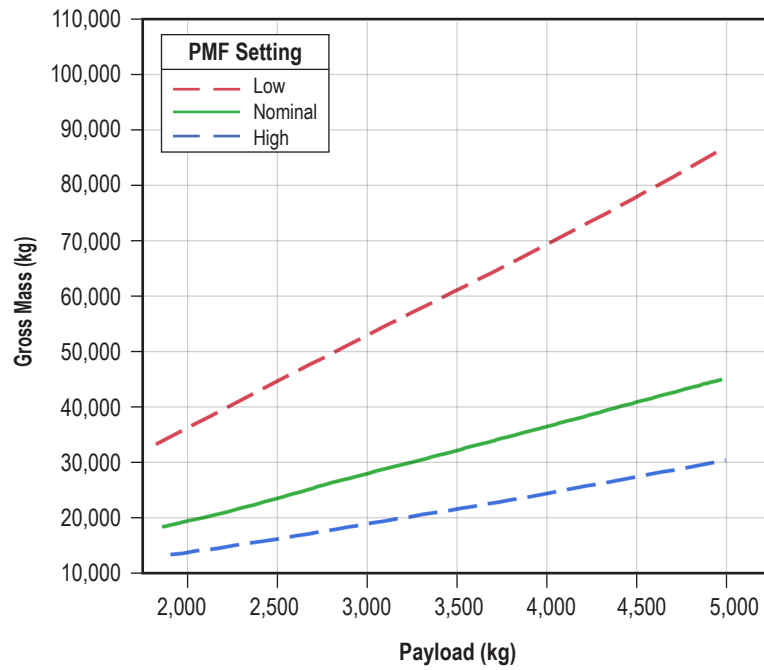


Figure 16. Payload versus gross mass for $I_{sp} = 360$ s, latitude = 30° , and orbit = 5 Sol.

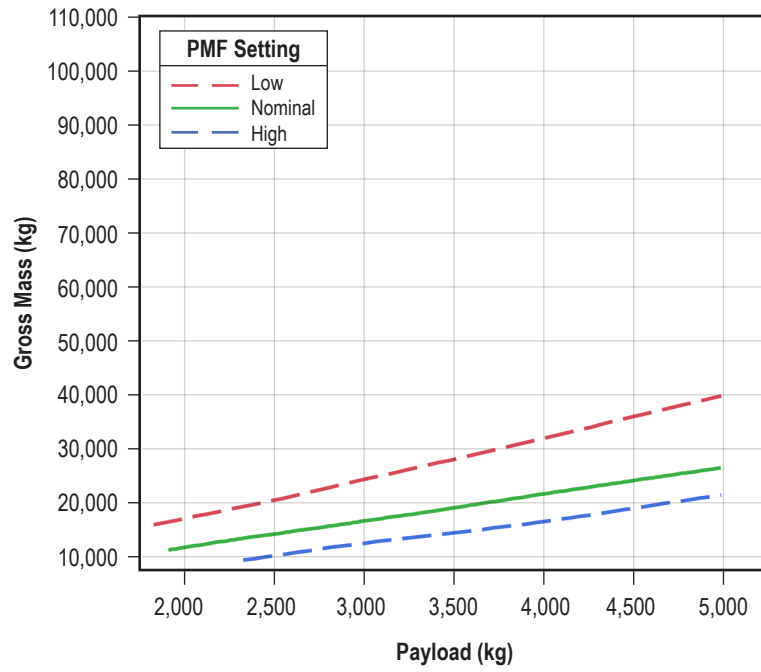


Figure 17. Payload versus gross mass for $I_{sp} = 360$ s, latitude = 30° , and orbit = 5 Sol.

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